Amendments to the Specification:

Please replace paragraph [0034], beginning at page 16, line 18 through page 17, line 20, with the following amended paragraph:

[0034] If the structure and location of the protein's binding site are not known (the NO branch of step 215), the method predicts that information as follows. Using the protein structural information, the method identifies a set of potential ligand binding sites by mapping the empty volumes available for ligand binding in the protein (step 220). The total volume available for docking is divided into small binding regions. Initial conformations for one or more ligands known to bind the protein are generated for each of the potential binding areas (step 225) using known techniques, such as the well-known DOCK 4.0 package, T.A. Ewing, et al. (1997) J. Comput. Chem. 18, 1175-1189, ~~which is incorporated by reference herein (DOCK 4.0 is available at http://www.cmpharm.ucsf.edu/kuntz/),~~ or any other publicly-available docking software. A set of best conformations (e.g. from about 1% to about 20% or more of the initial conformations identified in step 225, depending on the particular application) is selected for each of the known ligands in each potential binding area (step 230). These conformations are then optimized using molecular mechanics (step 235). The best of these conformations (i.e., those having the lowest energy scores) are identified and a probable binding site is identified based on the spatial clustering of the best conformations (step 240). Optionally, an additional selection criteria based on the percentage of the ligand surface area buried within the protein can be applied prior to the selection of lowest energy conformations. This probable binding site is used in the following steps.